CLAIMS:

What is claimed is:

1. A method, comprising:

(A) defining a first experimental space comprising factors of at least two mixtures with at least one common factor;

(B) defining a second experimental space by deleting duplicate factor combinations from said first experimental space; and

(C) conducting an experiment on said second experimental space.

2. The method of claim 1, wherein (C) comprises effecting a combinatorial high throughput screening (CHTS) to select a best case set of factors from said second experimental space.

3. The method of claim 2, wherein said CHTS comprises effecting parallel chemical reactions of an array of reactants defined by said second experimental space.

4. The method of claim 2, wherein said CHTS comprises effecting parallel chemical reactions on a micro scale on reactants defined as said second experimental space.

5. The method of claim 2, wherein (C) comprises an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating said identified products after completion of a single or repeated iteration.

6. The method of claim 1, wherein said second experimental space is defined by two or more factors, each having a plurality of possible identities.

7. The method of claim 1, wherein said second experimental space factors comprise reactants, catalysts and conditions and said (C) comprises (a) reacting a reactant selected from the second experimental space under a set of catalysts or

reaction conditions selected from the second experimental space and (b) evaluating a set of products of the reacting step and further comprising (D) reiterating step (C) wherein a next second experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step (C).

8. The method of claim 7, comprising reiterating (C) until a best set of factors of said second experimental space is selected.

9. The method of claim 1, wherein said first experimental space includes a catalyst system comprising combinations of Group IVB, Group VIB and Lanthanide Group metal complexes.

10. The method of claim 1, wherein said second experimental space includes a catalyst system comprising a Group VIII B metal.

11. The method of claim 1, wherein said second experimental space includes a catalyst system comprising palladium.

12. The method of claim 1, wherein said second experimental space includes a catalyst system comprising a halide composition.

13. The method of claim 1, wherein said second experimental space includes an inorganic co-catalyst.

14. The method of claim 1, wherein said second experimental space includes a catalyst system that includes a combination of inorganic co-catalysts.

15. The method of claim 1, wherein said second experimental space is a ternary space comprising a number of experiments defined by

$$V + \prod_{i=1}^{3} n_i \times I_3 + \left[\sum_{i=1}^{3} \frac{1}{n_i} \prod_{i=1}^{3} n_i \right] \times I_2$$

16. The method of claim 1, wherein said second experimental space is a quaternary space comprising a number of experiments defined by

$$V+\prod_{i=1}^{4} n_i \times I_4+\left[\sum_{i=1}^{4}\frac{1}{n_i}\prod_{i=1}^{4} n_i\right]\times I_3+\left[\sum_{i=1}^{4}\sum_{j=i+1}^{4}\frac{1}{n_i n_j}\prod_{i=1}^{4} n_i\right]\times I_2$$

17. The method of claim 1, wherein said second experimental space is a pentanary space comprising a number of experiments defined by

$$V+\prod_{i=1}^{5} n_i \times I_5 + \left[\sum_{i=1}^{5}\frac{1}{n_i}\prod_{i=1}^{5} n_i\right]\times I_4 + \left[\sum_{i=1}^{5}\sum_{j=i+1}^{5}\frac{1}{n_i n_j}\prod_{i=1}^{5} n_i\right]\times I_3 +$$

$$\left[\sum_{i=1}^{5}\sum_{j=i+1}^{5}\sum_{k=j+1}^{5}\frac{1}{n_i n_j n_k}\prod_{i=1}^{5} n_i\right]\times I_2$$

18. A system for selecting a best case set of experiments of a experimental reaction, comprising:

a processor that (A) defines a first experimental space comprising factors of at least two mixtures with at least one common factor and (B) defines a second experimental space by deleting duplicate factor combinations from said first experimental space; and

a reactor and evaluator to select a best case set of factors from said experimental space by a combinatorial high throughput screening (CHTS) method to select a best case set of factors from said experimental space.

19. The system of claim 18, wherein said processor comprises

a display terminal having screen displays whereby a researcher can input values for factors on said screen;

a database for storing said factors;

a computer for generating a set of test cases for a set of said factors based on a researcher specified value for identifying a number of interacting relationships within said factors;

a computer combining said test cases for set of factors with said relationships and providing a merged table of test cases; and

an output for writing to a database said merged table of test cases.

20. The system of claim 18, wherein said second experimental space is a ternary space comprising a number of experiments defined by

$$V + \prod_{i=1}^{3} n_i \times I_3 + \left[\sum_{i=1}^{3} \frac{1}{n_i} \prod_{i=1}^{3} n_i\right] \times I_2$$

21. The system of claim 18, wherein said second experimental space is a quaternary space comprising a number of experiments defined by

$$V + \prod_{i=1}^{4} n_i \times I_4 + \left[\sum_{i=1}^{4} \frac{1}{n_i} \prod_{i=1}^{4} n_i\right] \times I_3 + \left[\sum_{i=1}^{4} \sum_{j=i+1}^{4} \frac{1}{n_i n_j} \prod_{i=1}^{4} n_i\right] \times I_2$$

22. The system of claim 18, wherein said second experimental space is a pentanary space comprising a number of experiments defined by

$$V + \prod_{i=1}^{5} n_i \times I_5 + \left[\sum_{i=1}^{5} \frac{1}{n_i} \prod_{i=1}^{5} n_i\right] \times I_4 +$$

$$\left[\sum_{i=1}^{5} \sum_{j=i+1}^{5} \frac{1}{n_i n_j} \prod_{i=1}^{5} n_i\right] \times I_3 + \left[\sum_{i=1}^{5} \sum_{j=i+1}^{5} \sum_{k=j+1}^{5} \frac{1}{n_i n_j n_k} \prod_{i=1}^{5} n_i\right] \times I_2 .$$

23. An experimental space, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{t=1}^{T} n_t \cdot I_T + \left(\sum_{t=1}^{T} \frac{1}{n_t}\right) \times \left(\prod_{t=1}^{T} n_t\right) \times [I_{(T-1)}]$$

for a ternary system ($T = 3$) or an algorithm for a succeeding T-nary system, determined from a previous term by:(a) adding an additional term which contains an additional summation, incremented over a next index from a starting point one unit

higher than the first summation ; (b) decrementing the subscript on ***I*** ; and (c) adding a value of n, indexed by the next index, to the inverse term.

24. The experimental space of claim 23, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^{4} n_i \times I_4 + \left[\sum_{i=1}^{4} \frac{1}{n_i} \prod_{i=1}^{4} n_i\right] \times I_3 + \left[\sum_{i=1}^{4} \sum_{j=i+1}^{4} \frac{1}{n_i n_j} \prod_{i=1}^{4} n_i\right] \times I_2$$

for a quaternary system.

25. The experimental space of claim 23, comprising a number of mixture combinations defined by an algorithm, which expresses the sum of terms:

$$V + \prod_{i=1}^{5} n_i \times I_5 + \left[\sum_{i=1}^{5} \frac{1}{n_i} \prod_{i=1}^{5} n_i\right] \times I_4 +$$

$$\left[\sum_{i=1}^{5} \sum_{j=i+1}^{5} \frac{1}{n_i n_j} \prod_{i=1}^{5} n_i\right] \times I_3 + \left[\sum_{i=1}^{5} \sum_{j=i+1}^{5} \sum_{k=j+1}^{5} \frac{1}{n_i n_j n_k} \prod_{i=1}^{5} n_i\right] \times I_2$$

for a pentanary system.